

Entanglement signatures of the quantum phase transition induced by a magnetic impurity in a superconductor

P. D. Sacramento^{1,2}, P. Nogueira², V. R. Vieira^{1,2} and V. K. Dugaev^{1,2,3}

¹*Departamento de Física and* ²*Centro de Física das Interações Fundamentais,*

Instituto Superior Técnico,

Universidade Técnica de Lisboa (TULisbon),

Av. Rovisco Pais, 1049-001 Lisboa, Portugal

³*Department of Mathematics and Applied Physics,*

Rzeszów University of Technology,

Al. Powstańców Warszawy 6, 35-959 Rzeszów, Poland

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The insertion of a magnetic impurity in a superconductor induces a first order quantum phase transition as the coupling to the electronic spin density increases. As the transition is crossed, a discontinuity is exhibited by various quantities, like the total spin density, the total gap function and the gap function at the impurity location. The location of other quantum phase transitions have been detected by singularities in entanglement measures of the system. In this work we show that the single-site and two-site von Neumann entropies, the mutual information and the Meyer-Wallach measure show discontinuities at the quantum phase transition. The negativity is less sensitive to the transition. We study in detail these quantities as a function of spin coupling and distance from the impurity center.

I. INTRODUCTION AND MODEL

There has been in recent years a very rich interplay between quantum information and computation and the study of quantum many-body systems¹.

The concept of entanglement of quantum states — which was introduced by Schrödinger², already in 1935, at the time of the EPR paradox³, and latter explored by Bell⁴ to establish his famous inequalities — has been a crucial factor in the impressive developments in the area of quantum information and computation. This made possible the distinction between quantum and classical physics on an operational basis, leading to the experimental confirmation^{5,6,7} of quantum mechanics.

The development of the formalism and techniques used in the area of quantum information and computation⁸ has occurred in parallel with developments in other scientific areas, with each area being a source of inspiration to each other. The study of quantum many-body systems and their correlations and phase transitions, both at zero and non-zero temperatures, provides an unambiguous example of that mutual influence.

One example is the development of the Matrix Product States (MPS)⁹ and of the Projected Entangled-Pair States (PEPS)¹⁰, which provide an efficient calculation of the low-lying energy states of quantum systems, and the reformulation^{11,12} of the density matrix renormalization group (DMRG)¹³, allowing to understand and overcome some of its limitations, associated to the boundary conditions in the system.

This interrelation has also been explored in the reanalysis of several non-trivial exactly solvable models, under the new methods and concepts, using the known ground state or correlation functions to calculate the different information measures and to better understand the underlying physics. These models are typically either one dimensional spin^{14,15} or electron chains^{16,17}, solvable by the Bethe ansatz or the Jordan-Wigner and the Bogoliubov-Valatin transformations, or effectively infinite dimensional models, where each particle interacts equally with all the others^{18,19}. Intermediate dimensions or extensions of these models have also been studied usually using numerical methods.

For a bipartite system, in particular for a two qubit system, the entanglement measures are well established and essentially equivalent. However, this is not the case for systems with a larger number of components²⁰. The issue is even complicated by the restrictions on how to share entanglement by more than two particles, the so-called monogamy of entanglement²¹. Besides the von Neumann and related quantities⁸, other information measures like the concurrence²², the negativity²³ or the Meyer-Wallach²⁴ and the generalized global entanglement measures²⁵ have been considered.

In most discussions on entanglement, the particles constituting the systems are considered distinguishable. The Schmidt rank, central in this analysis, assumes this, for example. However, this is not the case for the quantum statistics, obeyed by the fermions and bosons, and new methods have to be used¹. The effect of the quantum statistics has been analyzed for free electrons²⁶ and bosons²⁷, and for electrons in a BCS superconductor²⁸ or with the so called eta-pairing²⁹.

In this work we consider the quantum phase transition induced by a magnetic impurity inserted in a conventional superconductor^{30,31,32,33,34,35,36,37}, and study it using some of those entanglement measures as a signature of the quan-

tum phase transition. Consider a classical spin immersed in a two-dimensional s -wave conventional superconductor. We use a lattice description of the system. In the center of the system ($i = l_c = (x_c, z_c)$) we place a classical spin parametrized like

$$\frac{\vec{S}}{S} = \cos \varphi \vec{e}_x + \sin \varphi \vec{e}_z \quad (1)$$

where S is the modulus of the spin. We assume that the spin lies in the plane of the superconducting film ($x - z$ plane). The Hamiltonian of the system is given by

$$\begin{aligned} H = & - \sum_{\langle i,j \rangle, \sigma} t_{i,j} c_{i\sigma}^\dagger c_{j\sigma} - e_F \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + \sum_i \left(\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \Delta_i^* c_{i\downarrow} c_{i\uparrow} \right) \\ & - \sum_{\sigma, \sigma'} J_{l_c} [\cos \varphi c_{l_c\sigma}^\dagger \sigma_{\sigma, \sigma'}^x c_{l_c\sigma'} + \sin \varphi c_{l_c\sigma}^\dagger \sigma_{\sigma, \sigma'}^z c_{l_c\sigma'}], \end{aligned} \quad (2)$$

where the first term describes the hopping of electrons between different sites on the lattice, e_F is the chemical potential, the third term is the superconducting s -pairing with the site-dependent order parameter Δ_i , and the last term is the exchange interaction of an electron at site $i = l_c$ with the magnetic impurity. The hopping matrix is given by $t_{i,j} = t \delta_{j, i+\delta}$ where δ is a vector to a nearest-neighbor site. Note that both the indices l and i, j specify sites on a two-dimensional system. The indices $i, j = 1, \dots, N$, where N is the number of lattice sites.

Since the impurity spin acts like a local magnetic field the electronic spin density will align along the local field. For small values of the coupling there is a negative spin density around the impurity site. At the impurity site it is positive, as expected. For larger couplings the spin density in the vicinity of the impurity site is positive. At small couplings the many-body system screens the effect induced by the impurity inducing fluctuations that compensate the effect of the local field in a way that the overall magnetization vanishes. However, for strong enough coupling the many-body system becomes magnetized in a discontinuous fashion. One interpretation is that if J is strong enough the impurity breaks a Cooper pair and captures one of the electrons, leaving the other electron unpaired, and thus the overall electronic system becomes polarized. The impurity induces a pair of bound states inside the superconducting energy gap, one at positive energy (with respect to the chemical potential), and another at a symmetric negative energy. Even though the spectrum is symmetric the spectral weights of the two energy levels are not the same and their spin content is also distinct. The analysis of the local density of states (LDOS)^{34,38} shows that for small coupling the lowest positive energy level has only a contribution from spin \uparrow and the first level with negative energy (symmetric to the other level) has only contribution from spin \downarrow . The magnitude of the spectral weight at the impurity site is different for the two states. Considering now the second level located in the continuum, both at positive and negative energies, there is a mixture of both spin components, even though in the case of the state at positive energy the magnitude of the peak is larger for the case of spin \uparrow than for the case of spin \downarrow and in the case of the state in the continuum at negative energy the relative magnitudes of the two spin components are reversed. Considering a higher value for the coupling one finds that the levels inside the gap approach the Fermi level. There is a critical value of the coupling for which the two levels cross in a discontinuous way such that it coincides with the emergence of a finite overall magnetization. After the level crossing has occurred, the nature of the states changes. The positive energy bound state has now only a contribution from the spin \downarrow component and vice-versa, the first negative energy state has only contribution from the spin component \uparrow . As the level crossing occurred the spin content has changed. On the other hand, in the first state in the continuum, where the two spin components contribute, the magnitude of the \uparrow component is now much larger than the \downarrow component while for a smaller value of the coupling the magnitudes were of similar size. Also, the \downarrow component of the second state of negative energy is now much smaller than the \uparrow component. The second state has to compensate for the spin flip of the lowest state by increasing the weight of the spin component aligned with the external impurity spin.

The diagonalization of this Hamiltonian is performed using the Bogoliubov-Valatin transformation in the form

$$\begin{aligned} c_{i\uparrow} &= \sum_n [u_n(i, \uparrow) \gamma_n - v_n^*(i, \uparrow) \gamma_n^\dagger] \\ c_{i\downarrow} &= \sum_n [u_n(i, \downarrow) \gamma_n + v_n^*(i, \downarrow) \gamma_n^\dagger] \end{aligned} \quad (3)$$

Here n is a complete set of states, u_n and v_n are related to the eigenfunctions of Hamiltonian (2), and the new fermionic operators γ_n are the quasiparticle operators. These are chosen such that in terms of the new operators

$$H = E_g + \sum_n \epsilon_n \gamma_n^\dagger \gamma_n \quad (4)$$

where E_g is the ground state energy and ϵ_n are the excitation energies. As a consequence

$$\begin{aligned} [H, \gamma_n] &= -\epsilon_n \gamma_n \\ [H, \gamma_n^\dagger] &= \epsilon_n \gamma_n^\dagger \end{aligned} \quad (5)$$

The coefficients $u_n(i, \sigma)$, $v_n(n, \sigma)$ can be obtained solving the Bogoliubov-de Gennes (BdG) equations³⁹. Defining the vector

$$\psi_n(i) = \begin{pmatrix} u_n(i, \uparrow) \\ v_n(i, \downarrow) \\ u_n(i, \downarrow) \\ v_n(i, \uparrow) \end{pmatrix}$$

the BdG equations can be written as

$$\mathcal{H}\psi_n = \epsilon_n \psi_n \quad (6)$$

where the matrix \mathcal{H} at site i is given by

$$\mathcal{H} = \begin{pmatrix} -h - e_F - J_{lc} \sin \varphi & \Delta_i & -J_{lc} \cos \varphi & 0 \\ \Delta_i^* & h + e_F - J_{lc} \sin \varphi & 0 & -J_{lc} \cos \varphi \\ -J_{lc} \cos \varphi & 0 & -h - e_F + J_{lc} \sin \varphi & \Delta_i \\ 0 & -J_{lc} \cos \varphi & \Delta_i^* & h + e_F + J_{lc} \sin \varphi \end{pmatrix}$$

where $h = t\hat{s}_\delta$ with $\hat{s}_\delta f(i) = f(i+\delta)$. The solution of these equations gives both the energy eigenvalues and eigenstates. The problem involves the diagonalization of a $(4N) \times (4N)$ matrix. The solution of the BdG equations is performed self-consistently imposing at each iteration that

$$\Delta_i = \frac{g}{2} [\langle c_{i\uparrow} c_{i\downarrow} \rangle - \langle c_{i\downarrow} c_{i\uparrow} \rangle] \quad (7)$$

where g is the effective attractive interaction between the electrons. Using the canonical transformation this can be written as

$$\begin{aligned} \Delta_i &= -g \sum_{n, 0 < \epsilon_n < \hbar\omega_D} \{ f_n (u_n(i, \uparrow) v_n^*(i, \downarrow) + u_n(i, \downarrow) v_n^*(i, \uparrow)) \\ &\quad - \frac{1}{2} [u_n(i, \uparrow) v_n^*(i, \downarrow) + u_n(i, \downarrow) v_n^*(i, \uparrow)] \} \end{aligned} \quad (8)$$

where ω_D is the Debye frequency, and f_n is the Fermi function defined as usual like

$$f_n = \frac{1}{e^{\epsilon_n/T} + 1}$$

where T is the temperature. We note that the Bogoliubov-de Gennes equations are invariant under the substitutions $\epsilon_n \rightarrow -\epsilon_n$, $u(\uparrow) \rightarrow v(\uparrow)$, $v(\uparrow) \rightarrow u(\uparrow)$, $v(\downarrow) \rightarrow -u(\downarrow)$, $u(\downarrow) \rightarrow -v(\downarrow)$.

II. VON NEUMANN ENTROPY

Consider a system at zero temperature so that its density matrix respects the ground state. If this is a pure state, as in our problem, the density matrix is simply

$$\rho = |\Phi\rangle\langle\Phi| \quad (9)$$

where $|\Phi\rangle$ is the ground state, which in our case is the BCS ground state wave-function. Consider now that one can divide the system into two parts A and B, and define

$$\rho_A = \text{Tr}_B \rho. \quad (10)$$

This quantity characterizes the reduced density matrix of the subsystem A, having integrated out the degrees of freedom of the rest of the system, B. However, the information on the correlations intrinsic to part B and the

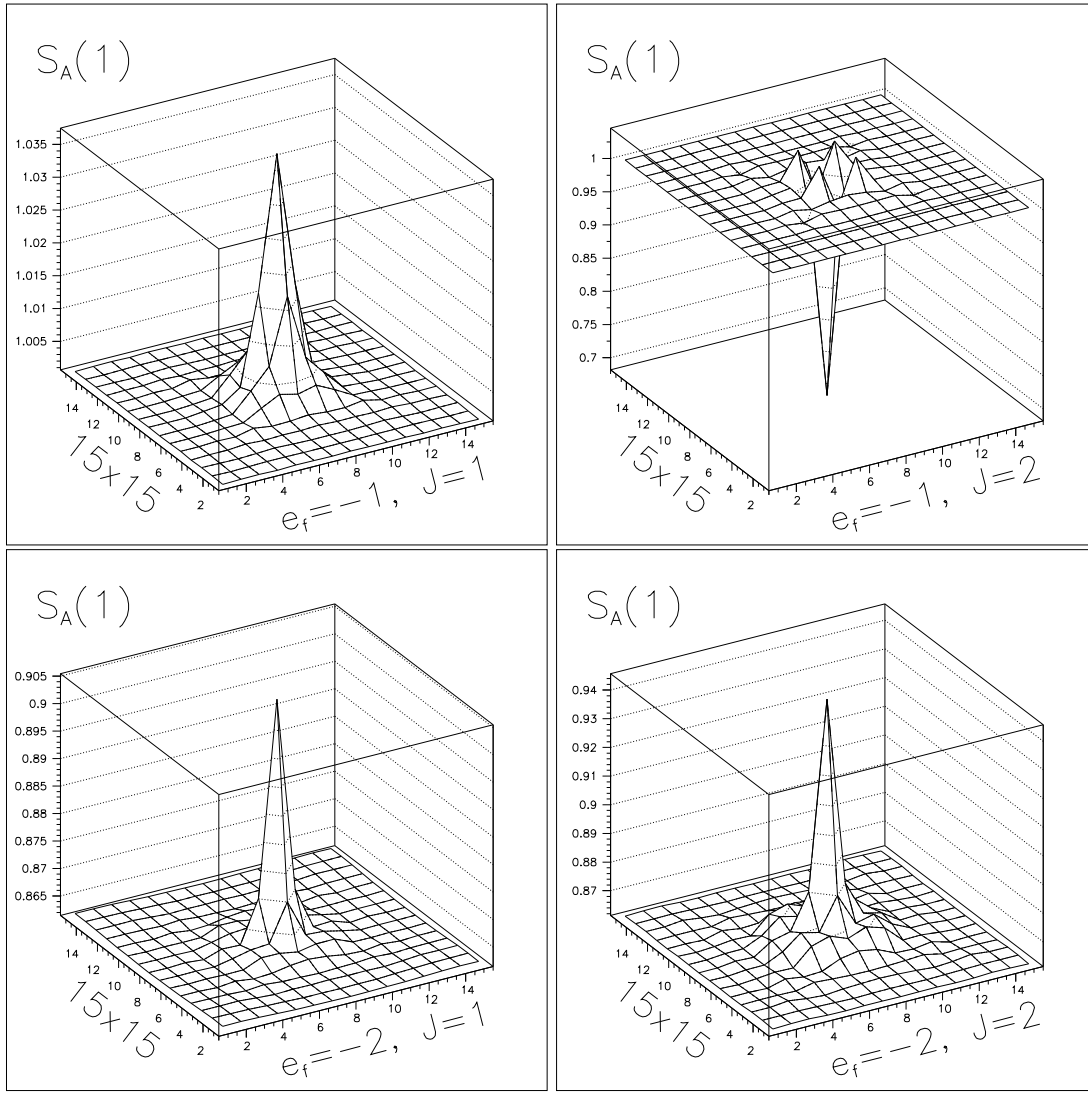


FIG. 1: Single-site von Neumann entropy $S_A(1)$ for $J = 1, 2$ and for different chemical potentials $e_F = -1, -2$. The system size is 15×15 . Note that in this figure and in the others the entropy is expressed in the basis e .

correlations between the two subsystems is implicit. We can therefore define the so-called von Neumann entropy as the information contained on part A of the system in the usual way

$$S_A = -\text{Tr} \rho_A \ln_2 \rho_A \quad (11)$$

This quantity is one possible measure of the entanglement between subsystem A and the rest of the system.

The subsystem A may have different extensions. The simplest case corresponds to select A as a single site and B the remaining $N - 1$ sites. In a translationally invariant system, the entropy S_A will be the same for every site, but in a non-homogeneous system, as in our problem, the entropy is site dependent, since the impurity breaks the translational invariance. As we will see below the von Neumann entropy is site dependent particularly in the vicinity of the impurity. Also, we will see that it depends on the spin coupling, particularly as the quantum phase transition is crossed. It is also interesting to look at the two-site entanglement where the subsystem A is now composed of two sites (arbitrarily selected from the lattice) and B are the remaining $N - 2$ sites. This quantity also shows a behavior that clearly identifies the phase transition.

In many-body systems a description in terms of wave functions is quite involved and second quantization is the natural way to perform any calculation. The density matrix is however easily defined in terms of states. It is also easily defined in terms of its matrix elements in some basis and this approach is indeed easy to implement using Fock states. It is easy therefore to show that the matrix elements of the density matrix are simply defined in terms of correlation functions of the whole system. For instance, in the case of the single-site entanglement it can be shown

that, using a basis of local states like $|0\rangle, |\uparrow, \downarrow\rangle, |\uparrow\rangle, |\downarrow\rangle$, which denote the four possible states — unoccupied, double occupied, singly occupied with an electron with spin \uparrow and singly occupied with an electron with spin \downarrow , respectively — the density matrix can be defined as

$$\rho_A = \begin{pmatrix} \langle(1-n_\uparrow)(1-n_\downarrow)\rangle & \langle c_\uparrow^\dagger c_\downarrow^\dagger \rangle & 0 & 0 \\ \langle c_\downarrow c_\uparrow \rangle & \langle n_\uparrow n_\downarrow \rangle & 0 & 0 \\ 0 & 0 & \langle n_\uparrow(1-n_\downarrow) \rangle & \langle c_\downarrow^\dagger c_\uparrow \rangle \\ 0 & 0 & \langle c_\uparrow^\dagger c_\downarrow \rangle & \langle (1-n_\uparrow)n_\downarrow \rangle \end{pmatrix}$$

The spin and charge parts decouple. The spin part couples the two spin orientations and the charge part couples the empty and doubly occupied cases. The diagonal terms of the matrix describe the number of empty sites, number of doubly occupied sites, the number of \uparrow spin sites and the number of \downarrow spin sites, respectively. This matrix is easily diagonalized and the von Neumann entropy obtained straightforwardly. The sum of the diagonal terms is equal to 1 due to normalization.

The correlation functions are easily solved using the representation of the electron operators in terms of the BdG quasiparticle operators. Specifically, we can write the single-site density matrix as

$$\rho = \sum_{n,m} |n\rangle \rho_{nm} \langle m| \quad (12)$$

where $|n\rangle, |m\rangle$ are the four states described above. Consider now an operator O defined in terms of creation and annihilation operators of the electrons, and evaluate

$$Tr\{O\rho\} = \sum_{n,m} \langle n|O|m\rangle \rho_{m,n}. \quad (13)$$

To determine the matrix element ρ_{nm} of the density matrix it is enough, by inspection, to find which operator O is such that only the matrix element $\langle n|O|m\rangle$ is non-zero. This will tell us which correlation function gives which matrix element of the density matrix. Alternatively, one can express the operator $|m\rangle\langle n|$ in terms of the creation and annihilation operators. The results for ρ_A are in the equation referred above.

These matrix elements are defined in the subspace of the states of one site. However, since we have integrated out all the other sites, we may now replace the matrix elements by the matrix elements over the entire system (direct product of the states of the remaining $N-1$ sites).

The case of the two-site entanglement is much more involved. One introduces two sites, i and j , and uses the same basis states for each site. The basis states are given by the direct product of these two basis sets and the reduced density matrix is now a 16×16 matrix. It is convenient to organize the basis states into even-even and odd-odd states in the number of electrons in the sites i and j , respectively. These two sets of states decouple and we are reduced to the diagonalization of two 8×8 matrices. The calculation of the various correlation functions involved in these two matrices would be rather lengthy if performed by hand. Note that one of the correlation functions involves the double occupancies at the two sites. This involves a product of eight electron operators, and each electron operator is given by a sum of two quasiparticle operators. Also one should pay special attention to the anti-commutators of the electron and quasiparticle operators. It is therefore advisable to calculate all of these correlation functions in an automatic way, using a symbolic algebra package, and we did so with the help of the computer program FORM⁴⁰.

A. Single-site von Neumann entropy

Let us consider the results for the single-site entropy. We will present results for a system of size 15×15 . As we have shown previously³⁸ the nature of the phase transition is not affected by changing either the system size or the boundary conditions (ie they can be either open or periodic). As shown previously, if the system is large enough the states induced by the impurity are localized and therefore not affected by the boundary. Also, since in this problem we are dealing with a first order quantum phase transition, not a second order one, there are no long range critical fluctuations that would imply a more careful scaling analysis. So we will limit ourselves to an adequate system size that illustrates the sensitivity of the entanglement measures to the ground state phase transition.

In Fig. 1 we show the results for the single-site entropy for different chemical potentials. In the case $e_F = -1$ the quantum phase transition is signaled by the change in the entropy near the impurity location. Below the QPT there is a maximum and as the QPT occurs the entropy develops a local minimum as the system gets correlated. Before the QPT is reached the impurity leads to a local increase of the entropy since it acts against the order due to the superconducting phase. At the QPT the physical picture is that the impurity locks an electron, which causes a local

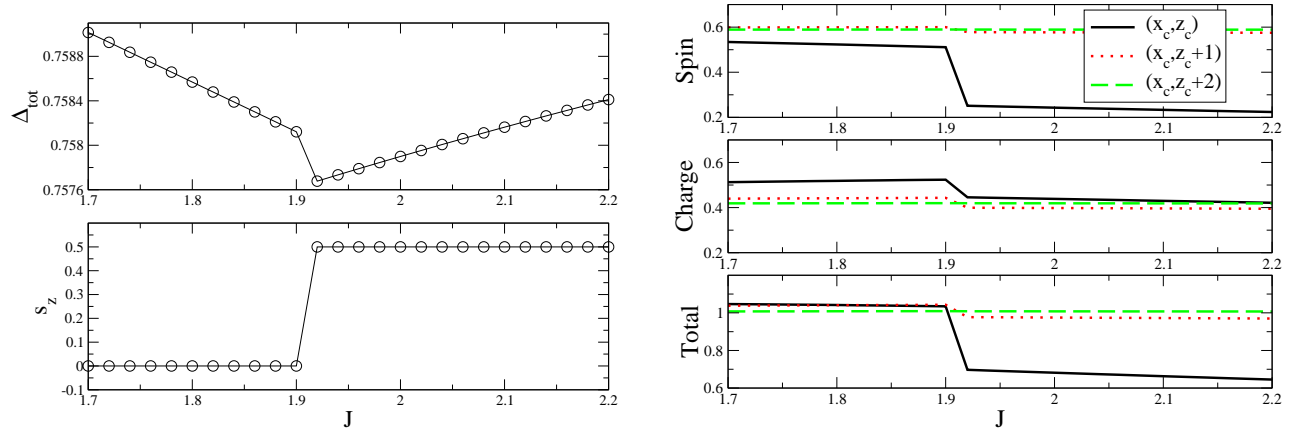


FIG. 2: a) Total gap function and spin magnetization and b) spin, charge and total contributions to the single-site entropy as a function of coupling. The curve in black corresponds to the impurity location, l_c , and the other two curves to two points distant by one lattice spacing and two lattice spacings. Notice the discontinuities signaling the QPT.

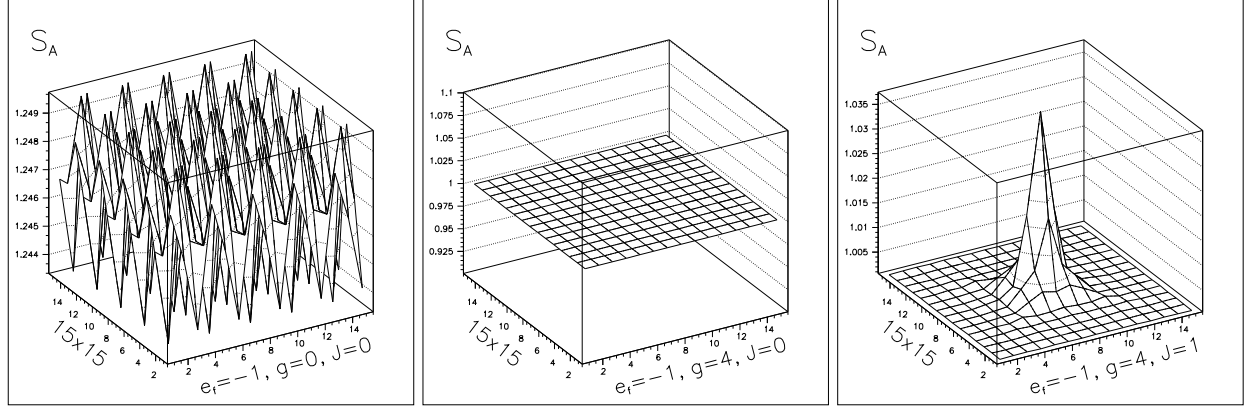


FIG. 3: Single-site entropy $S_A(1)$ for a tight-binding system ($g = 0, J = 0$), a superconductor ($g \neq 0, J = 0$) and a superconductor with a magnetic impurity ($g \neq 0, J = 1$).

decrease in entropy. In the case $e_F = -2$ a value of 2 for the coupling J is not strong enough to cross the phase transition.

In Fig. 2 we show the QPT signatures in terms of the total gap function and the total magnetization, and in terms of the single-site entropy. Notice that as the coupling increases the total magnetization becomes finite at the QPT, discontinuously, which is indicative of a first order phase transition. Note the small change on the average value of the gap function as the coupling changes. However, the trend is clearly altered as the QPT occurs. As the figure also shows, the largest entropy change is related to the spin degrees of freedom, as one might expect due to the spin interaction. However, as the trace of the reduced density matrix is normalized, the charge part is also discontinuous at the phase transition. It is also interesting to note that, as expected, at the impurity site, and for values of J higher than the critical value, the spin contribution to the entropy is smaller than the charge contribution.

In order to better clarify the meaning of the von Neumann entropy, in Fig. 3 we present a comparison of the single-site entanglement entropy for three different cases, namely i) a free (tight-binding) system where there is no superconductivity and no magnetic impurity, ii) a superconductor with no magnetic impurity, and iii) a superconductor with an impurity. The entropy is basically uniform in the free case and in the superconductor. The value in the free case is larger, as expected due to the ordered nature of the superconductor. Introducing the impurity changes the entropy in the vicinity of the impurity but does not alter the background value.

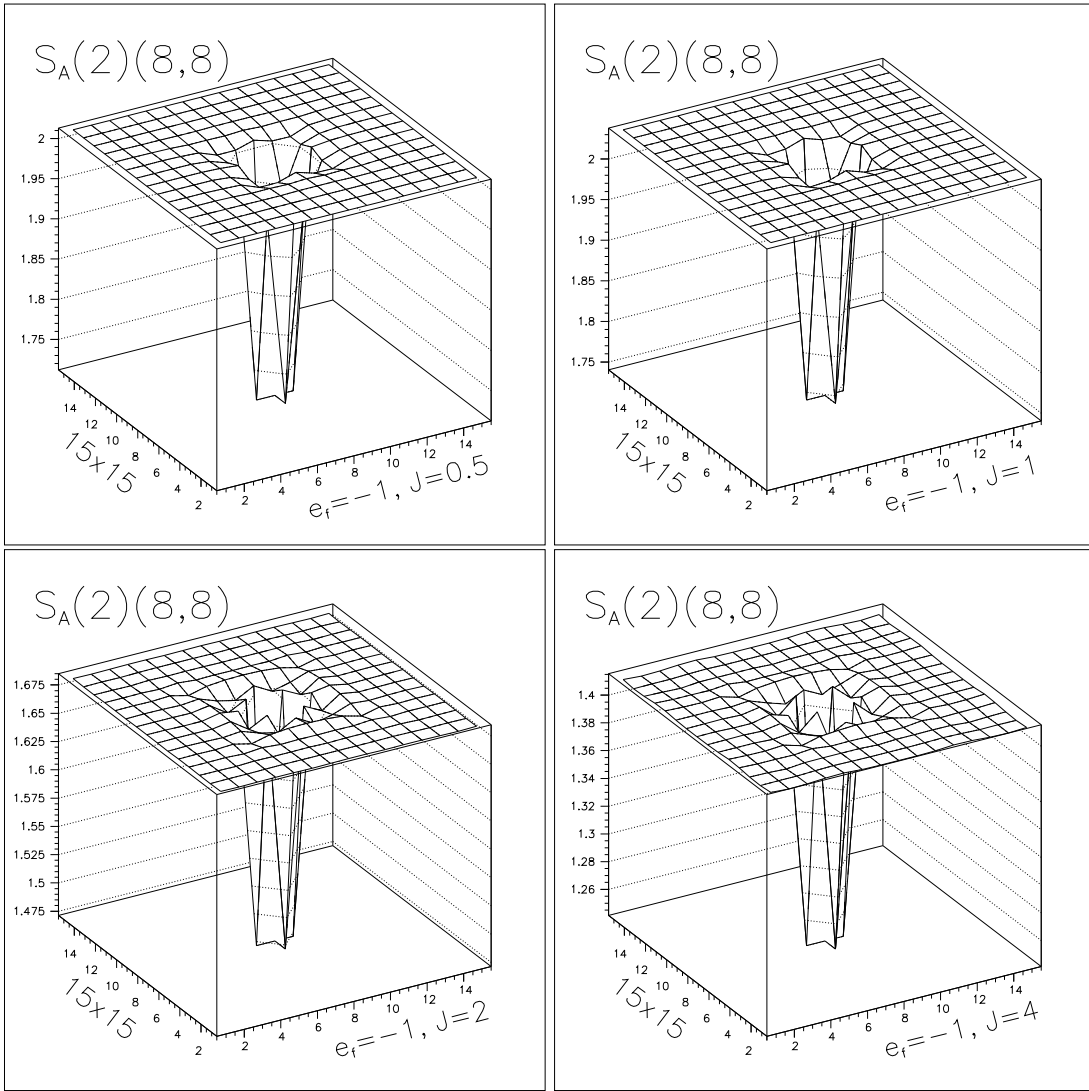


FIG. 4: Two-site entropy $S_A(2)$ where $i = (x_c, z_c) = (8, 8)$ is at the impurity location for a system with 15×15 sites and j is at any other location, for $J = 0.5, 1, 2, 4$.

B. Two-site von Neumann entropy

Consider now the two-site entanglement. The von Neumann entropy now measures the entanglement between two sites and the remaining $N - 2$ sites.

In Fig. 4 we present the two-site entanglement entropy choosing the spin impurity as a fixed site and letting the second site be any other site of the system. Notice the decrease in the entanglement entropy when the second site is in the vicinity of the fixed site. This is natural since one expects close neighbors to be more strongly correlated than further distanced sites, and therefore the entropy should be lower in the first case. Also, as the QPT transition is crossed, even though the structure of the two-site entanglement entropy is not strongly affected one may observe that the background value steadily decreases. This is consistent with the decrease of the single-site entanglement entropy in the vicinity of the impurity.

In Fig. 5 we present some results for the case where the fixed site is now in the bulk. Notice that as the coupling increases one can observe two structures: one related to the points in the vicinity of the bulk site, where the entropy is smaller, and another structure near the impurity site. Notice that in this case the background value is not affected when the QPT is crossed.

We may as well compare the two-site entropy for a free system, a superconductor, and a superconductor with the impurity inserted. For instance it is interesting to consider the case where one of the points of subsystem B is

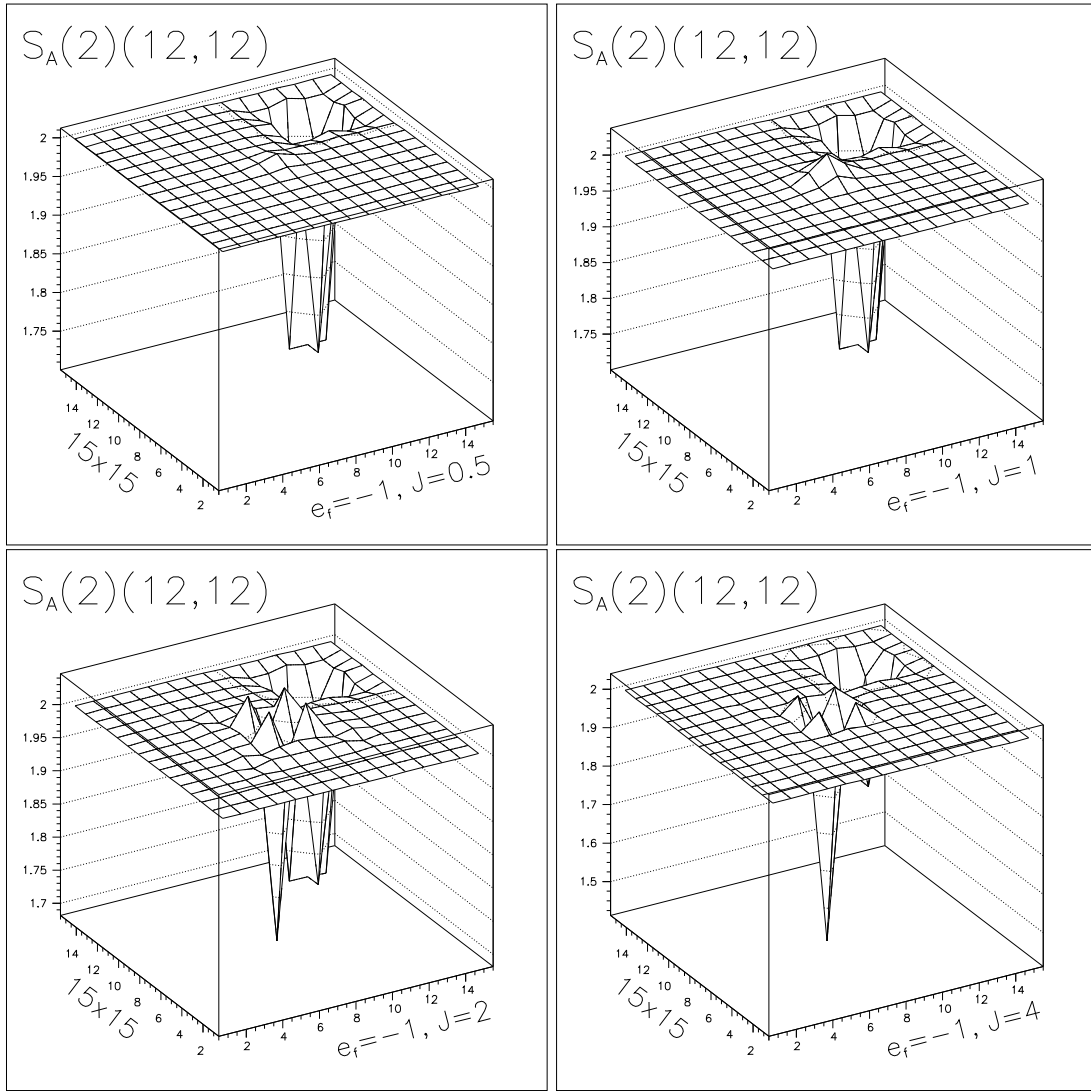


FIG. 5: Two-site entropy $S_A(2)$ where $i = (12, 12)$ is a site in the bulk and j is at any other location, for $J = 0.5, 1, 2, 4$.

the impurity site. In the tight-binding case one finds small ripples (as for the single-site entanglement) which are smoothened in the superconductor. Also, the background value decreases when the system becomes superconductor. In all cases there is a depression in the two-site entanglement when the points i and j are nearby. The effect of the impurity is to narrow somewhat the extent of that depression, which therefore becomes hardly noticeable. In Fig. 6 we compare the two-site entanglement when one of the sites is the impurity site and the other any other as compared to a case where neither includes the impurity site, including a nearest-neighbor. The results show that the effect of the impurity is noticeable since the background value is strongly affected.

The QPT can therefore be as well signaled by the two-site entanglement entropy. In Fig. 7 we show, as a function of the coupling J , the two-site entropy in two cases: i) between a site in the bulk and any other site in the system, and ii) between the impurity site and any other site in the system. There is a clear regime difference in both cases as the critical point is crossed.

C. Mutual information

The von Neumann entropy measures the entanglement between the subsystem A and the rest of the system, denoted subsystem B. However, looking at the entanglement between two sites of the system should provide us with a more detailed view. We may define the reduced density matrix of a subsystem of two sites, by integrating as

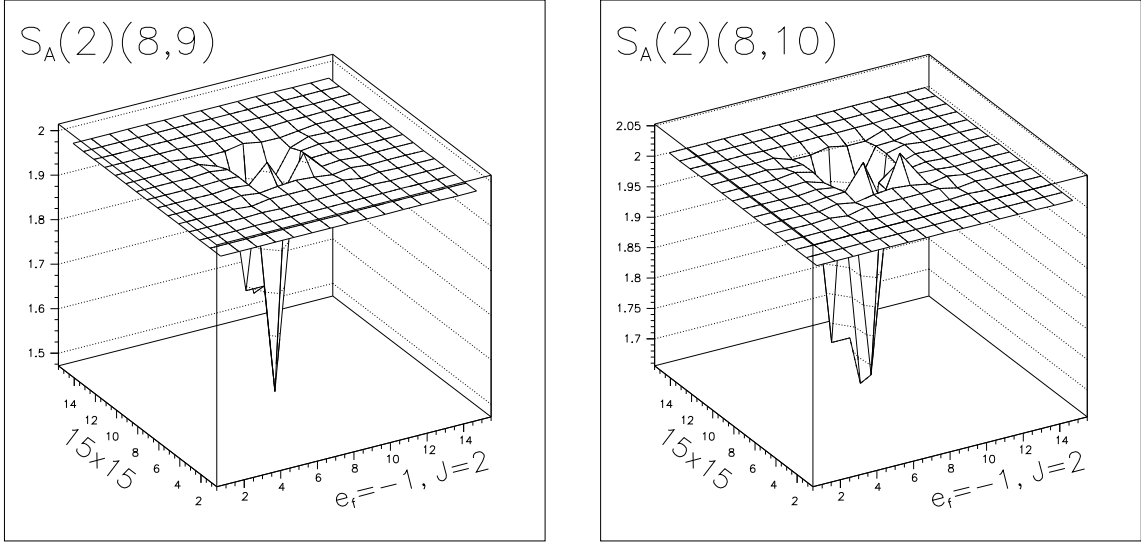


FIG. 6: Two-site entropy $S_A(2)$ for $J = 2$ where a) one of the points is fixed at a nearest-neighbor of the impurity and b) one of the points is fixed in the next-nearest-neighbor. Note that the background value is different with respect to the case where one of the points is fixed at the impurity.

before the degrees of freedom of the remaining $(N - 2)$ sites). We may now look at the entanglement between the two sites. In general the states between two sites may be divided into entangled and disentangled states. A subset of the disentangled states is given by the product states of the two sites. The entanglement between the two sites of subsystem A may be defined in the following way. The states are characterized by their density matrices. In a standard notation we will characterize the entangled states of two sites 1 and 2 by a density matrix ρ_{12} (which in our case is a reduced density matrix). A disentangled state that may be written as a product state is characterized by a density matrix η_{12} and a general disentangled state is characterized by a density matrix σ_{12} . The entanglement between the sites 1 and 2 is defined as the “distance”

$$E_{12} = \inf \text{Tr } \rho_{12} (\log \rho_{12} - \log \sigma_{12}) \quad (14)$$

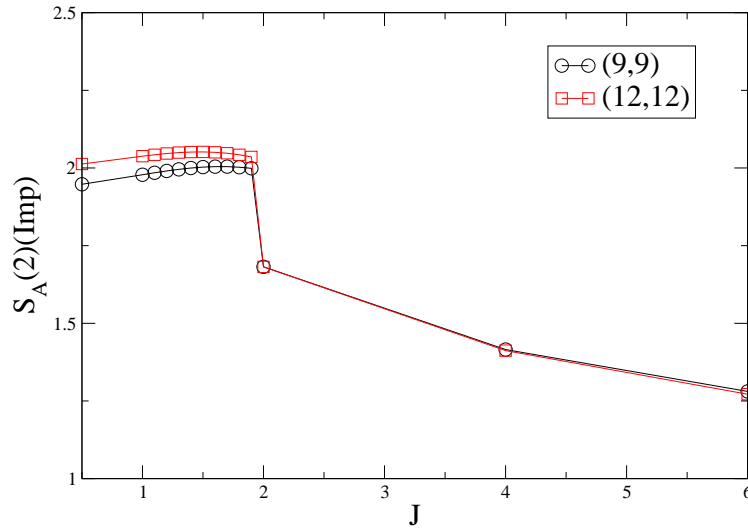


FIG. 7: Two-site entropy $S_A(2)$ as a function of J where one of the points is fixed at the impurity location and the other at another site in the bulk.

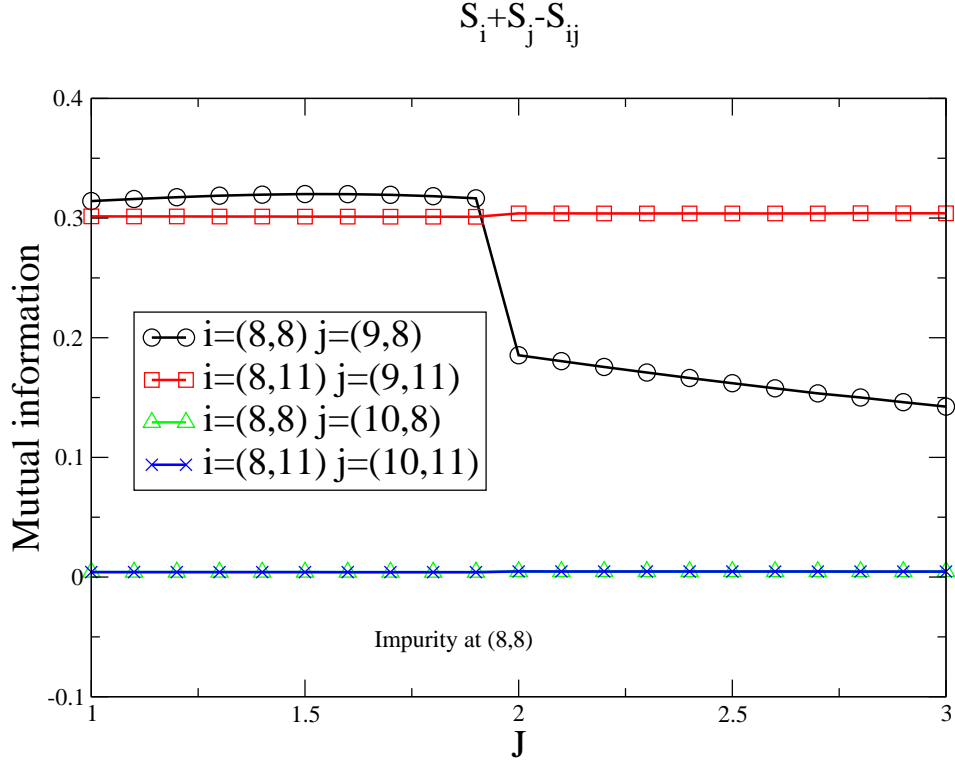


FIG. 8: Mutual information as a function of J where one of the points is fixed at the impurity location (8, 8) and the other at two sites in the bulk (9, 8), (10, 8) and one of the points is at a point in the bulk (8, 11) and two other points a nearest neighbor (9, 11) and a second nearest neighbor (10, 11).

The procedure to determine the infimum (minimum) of that trace is in general very complex. Another quantity that is much easier to calculate is the so-called mutual information where instead of looking for the “distance” over all disentangled states we just look for the minimum over the product states. This can be shown to lead to

$$M_{12} = S_A^{(1)}(1) + S_A^{(1)}(2) - S_A^{(2)}(1, 2) \quad (15)$$

where $S_A^{(1)}$ is a single-site von Neumann entropy and $S_A^{(2)}$ is a two-site von Neumann entropy. While E_{12} measures the full entanglement between the two sites, the mutual information just measures the correlation.

In Fig. 8 we compare the mutual information for different pairs of sites. When the sites are nearest neighbors the mutual information is finite and is otherwise quite small, even for second nearest neighbors. The QPT is clearly seen, particularly when one of the sites is the impurity site.

III. NEGATIVITY

Another quantity that has been proposed to distinguish between entanglement and non-entanglement is the so-called negativity. One considers two subsystems A and B, and constructs the joint density matrix of the two subsystems, call it ρ_{AB} . Define now the transposed in A density matrix in the sense that the basis states of part A are transposed while the basis states of part B remain the same. Looking at the eigenvalues of this new transposed density matrix one finds that it may have negative eigenvalues, even though the original density matrix never does. The existence of negative eigenvalues means that the system is necessarily entangled and therefore one possible measure of entanglement is the sum of the negative eigenvalues (which will be zero if the system is not entangled). In a fermionic many-body system there is always entanglement. However, as we have seen the extent of the entanglement changes as we turn on the superconductivity, introduce a magnetic impurity and change the spin coupling to the electronic spin density. We may expect therefore also some signature of the various transitions between these physical states and systems in the negativity. In our case we actually have a N site system (and a number of electrons given by the band-filling determined by the chemical potential). We construct a reduced two-site matrix integrating over $N - 2$ site degrees of freedom. These two sites, called above i and j may now take the role of A and B in the definition of the negativity.

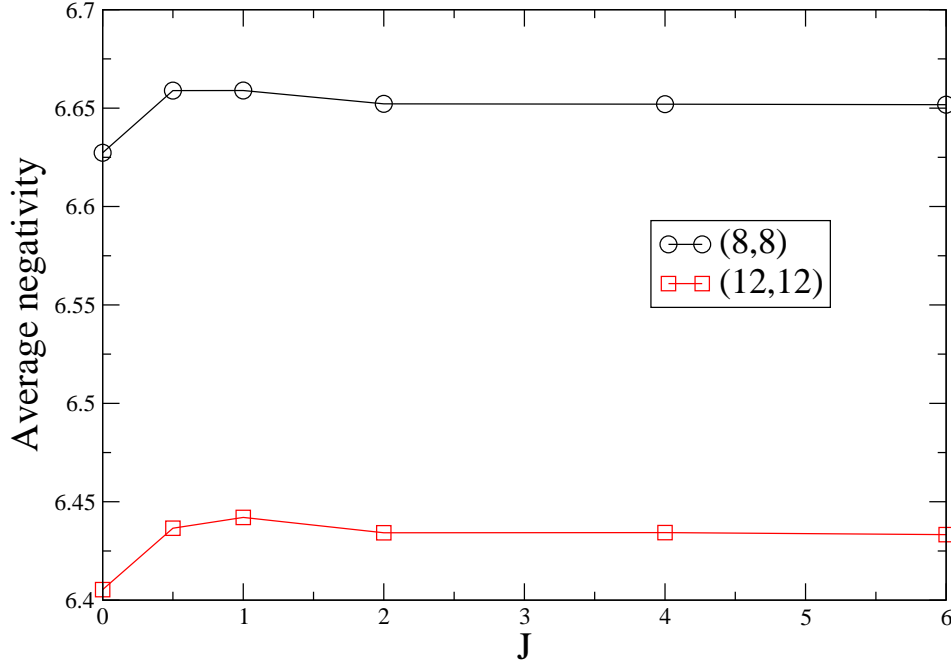


FIG. 9: Average negativity as a function of J where in one case one of the points is fixed at the impurity location and the other at a site in the bulk.

We can therefore define a corresponding transposed reduced density matrix where the basis states of for instance the i site (A subsystem) are transposed. We can relate the matrix elements of this transposed matrix to the matrix elements of the original reduced density matrix. We can as well determine its eigenvalues and calculate the negativity.

The negativity turns out to oscillate throughout the system. As we saw above, we could use the two-site entanglement entropy to detect the phase transition due to the effect of the transition on the entropy near the impurity location. However, as we saw this feature is small. While it is easily detectable in the case of the two-site entanglement entropy, the oscillations in the negativity are of the same order of magnitude and therefore not visible. However, as we saw the transition also affects the background value. We may therefore consider the average negativity throughout the system. This is shown in Fig. 9 where two cases are considered: one with the impurity as the fixed site and another with the fixed site in the bulk, both as a function of the spin coupling. In both cases we see that there is a slight change when the impurity is introduced ($J \neq 0$ with respect to the case of $J = 0$) and when the critical point is crossed. However the signature is quite small.

IV. MEYER-WALLACH MEASURE OR GENERALIZED GLOBAL ENTANGLEMENT

Another measure of entanglement is the so-called generalized global entanglement cited recently²⁵ as particularly suited to detect a QPT. It is defined like

$$G(2, n) = \frac{d}{d-1} [1 - \text{Tr}(\rho_{i,i+n}^2)] \quad (16)$$

where d is the dimensionality of the reduced density matrix (in our case $d = 16$) and the two-site density matrix refers to two points i and $j = i + n$. This quantity can be understood as the deviation of the reduced density matrix from the one of a pure state, where it would be zero. As referred in ref.²⁵ this measure is expected to be at least as good as the two-site entanglement entropy, analyzed above. The results for the function $G(2, n)$ are qualitatively the same as those for the two-site entropy, and we will not present them here in detail. When one of the sites, say i , is located at the impurity or at a bulk site the same features are found. When one of the sites is at the impurity site and the QPT is crossed there is a decrease in the background value and when one of the sites is located in the bulk for a value smaller than the critical value of J there is a small increase of the $G(2, n)$ at the impurity location and after the QPT is crossed there is a depletion, as for the two-site entropy.

It is however a good way to detect the phase transition if the results are presented in a clearer way (a similar role is achieved by the two-site entropy). Consider first the function $G(2, 1)$ and take $i = l_c = (8, 8)$. In Fig. 10 we show

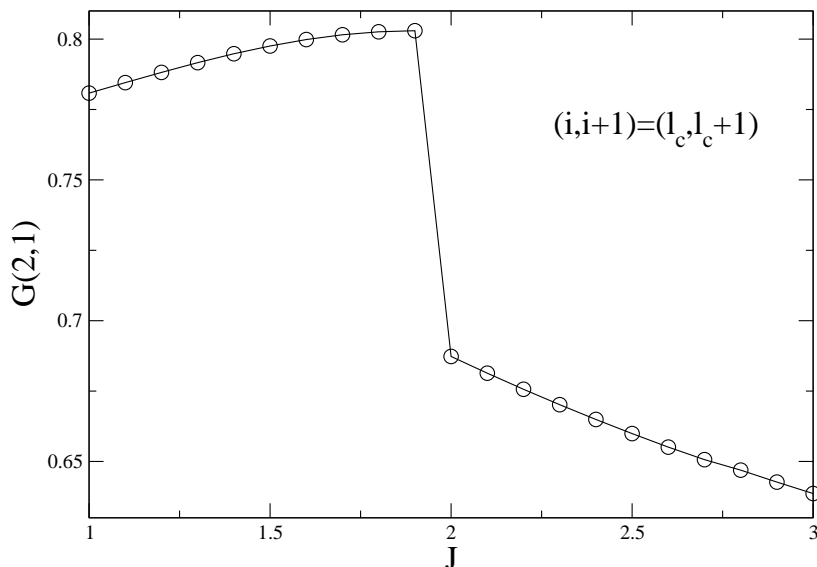


FIG. 10: Meyer-Wallach measure $G(2,1)$ as a function of J where one of the sites is at the impurity location and the other at a nearest neighbor. The QPT is clearly signaled.

the effect of changing the spin coupling J on this function. The QPT is clearly identified.

In Fig. 11 we show the dependence with distance of the generalized global entanglement function $G(2,n)$, where n is chosen along various directions fixing one of the points at the impurity location or a site in the bulk, for different spin couplings.

We conclude presenting the results for the same function $G(2,n)$ where the two sites i and $i+n$ define two lines that make an angle $\Phi = 0, \pi/2, \pi$ between themselves. We compare the cases where there is no impurity ($J = 0$) with the insertion of the impurity $J = 1, 2$. The influence of the impurity is noticed for small distances between the two sites and is particularly noted for the larger coupling. Interestingly, when the angle is large $\Phi = \pi$, which corresponds to the two sites involved in the entanglement being along the z axis with the impurity between them, the crossing of the QPT leads to a significant decrease of the function $G(2,n)$. This is shown in Fig. 12.

V. SUMMARY

In this work we have shown that various entanglement measures are suited to detect the quantum phase transition induced by a magnetic impurity inserted in a conventional s-wave superconductor. The magnetic impurity induces a pair of bound states that go through a level crossing as the coupling of the electronic spin density to the impurity spin grows. In this quantum phase transition the impurity locks an electron, thereby locally changing the spin density and the gap function, but it also changes the overall magnetization in a discontinuous manner. This transition is also easily detected for instance in the von Neumann entropy both for single-site and two-site subsystems. We have also considered the mutual information, the negativity, and the recently introduced generalized global entanglement. All quantities are sensitive to the change of the ground state of the system except for the negativity which is less accurate.

Since in the problem studied in this paper the single-site von Neumann entropy is separable into a spin part and a charge part (coupling empty sites and doubly occupied sites) we were able to show that the spin part is much more affected at the QPT, as expected. In agreement with the nature of the QPT, where an electron is captured by the impurity, the entropy at the impurity site decreases and since the physical state approaches a pure state the generalized global entanglement also decreases. Starting from a normal system (ie one with no impurities) and crossing the second order transition to the superconducting phase naturally leads to a decrease in entropy. The insertion of the impurity has a pair breaking effect and the entropy is locally increased. When the QPT is crossed the entropy decreases locally in the vicinity of the impurity, as stated above. We have also shown that the impurity and other sites are entangled, in the sense that the two-site von Neumann entropy is slightly lower when the impurity site is involved, irrespective of the distance between the impurity and the other site. However, this quantity is not a true measure of the direct correlation between the two sites. It is actually a measure of the entanglement of the two sites and the rest of the system. A better measure is the mutual information which is sensitive to the correlations between the two sites. This quantity has a rather short spatial range.

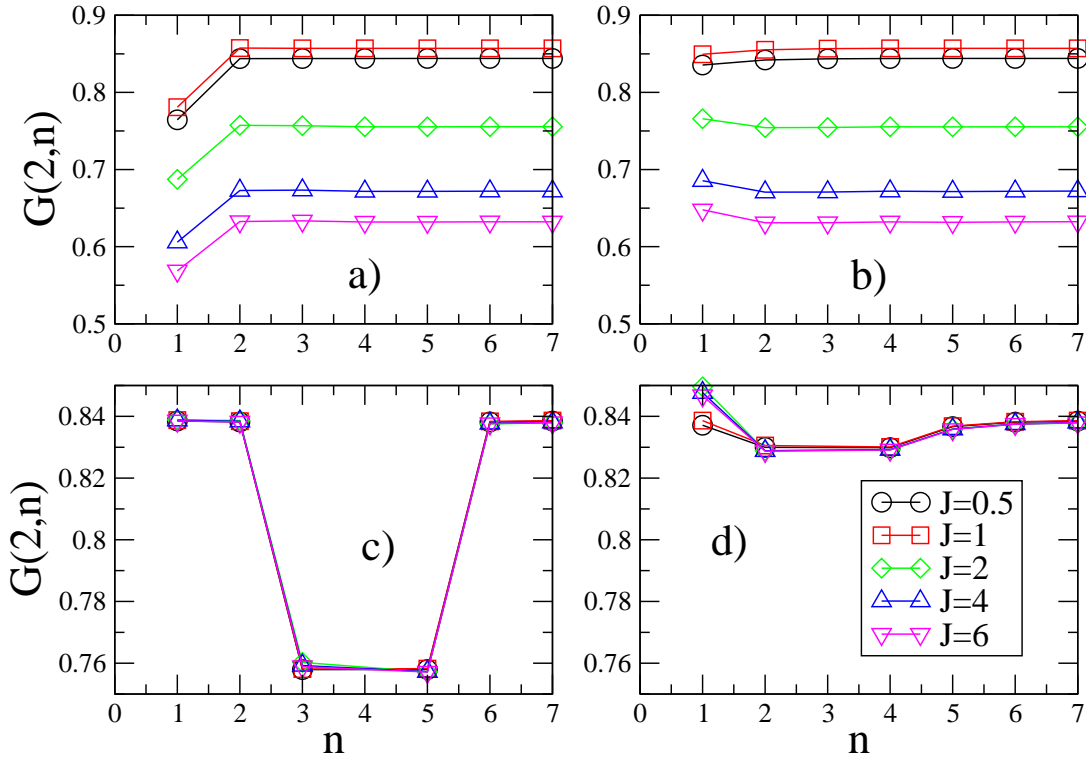


FIG. 11: $G(2, n)$ as a function of n for different spin couplings: the point i is fixed at the impurity location and a) n runs along the positive x direction and b) along the upper side of the diagonal $z = x$, and the point i is fixed at a bulk site located along the same diagonal with c) n along a horizontal line to the right of the impurity and d) the same diagonal from the impurity location to the right upper corner of the lattice.

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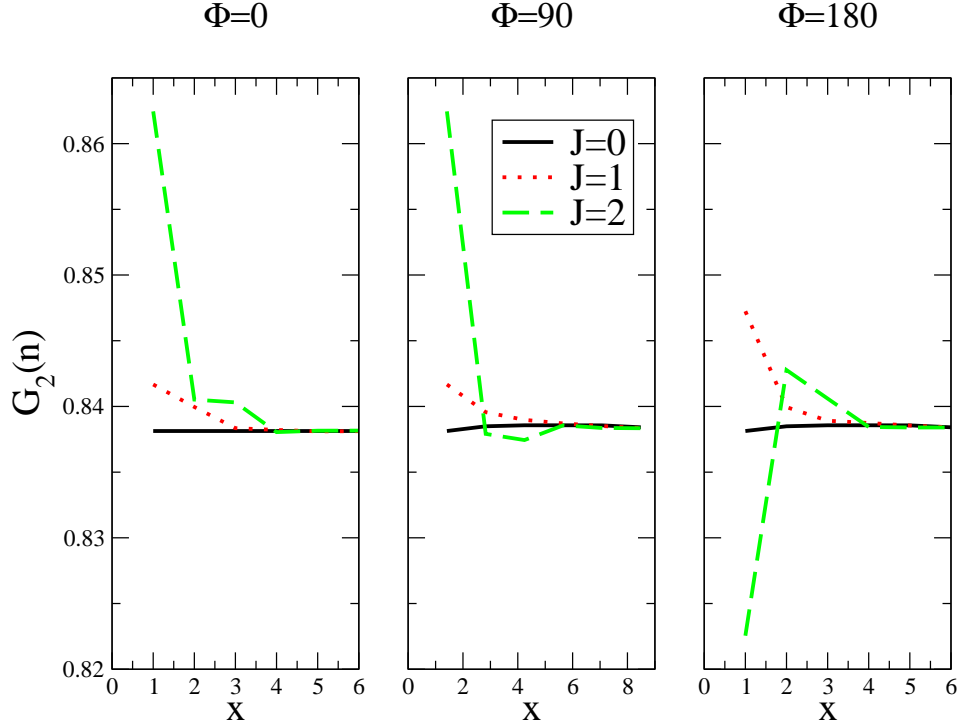


FIG. 12: $G(2, n)$ as a function of the distance to the impurity site for different spin couplings. The angle Φ is defined between the two lines over which the two sites involved in the entanglement are changing. The angle $\Phi = 0$ defines two parallel lines along the horizontal axis such that the distance between the two sites is fixed (in this case two lattice constants) but the distance of the pair to the impurity, x is increasing. The case $\Phi = \pi/2$ describes a situation where one of the sites is moving along the diagonal $z = x$ and the other along the diagonal $z = -x$ and finally the case $\Phi = \pi$ describes the case when one of the sites is moving along the vertical axis upward and the other point along the same axis but downward. Therefore, in the cases $\Phi = \pi/2, \pi$ the distance between the two points increasing while in the case $\Phi = 0$ it is constant. In all cases the distance x is the distance between one of the members of the pair and the impurity site.

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